OPTIMIZING THE MODELING PERFORMANCE FOR SAFETY ASSESSMENTS OF NUCLEAR WASTE REPOSITORIES BY APPROXIMATING TWO-PHASE FLOW AND TRANSPORT BY SINGLE-PHASE TRANSPORT SIMULATIONS

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ABSTRACT

The long-term safety performance of a potential deep geological repository for high-level and intermediate-level long-lived nuclear waste can be studied through numerical simulation tools capable of appropriately modeling the phenomenologies of interest in the repository and its environment. Because of the complexity of the modeled layout, the numerous physical processes, and the simulated times (up to 1 million years), computational needs are very high. TOUGH2-MP (Pruess et al. 1999, Zhang et al. 2008) is a suitable tool for modeling the impact that heat and gas generated in the emplacement areas may have on the evolution of fluid pressure and saturation fields in repository drifts and shafts (as well as in the host rock itself). The module EOS7R also enables the computing of coupled radionuclide transfer.

With respect to computational efficiency, it is useful to decouple transport from hydraulic calculations, for three primary reasons: (1) it allows using the hydraulic calculation once for several transport computations of a performance analysis and safety assessment (PA/SA) study, which is expected to lead to a substantial gain in CPU time; (2) it allows for optimizing the discretization separately for both hydraulic and transport calculations; and (3) it also allows for combining the TOUGH2 hydraulic and other codes modeling radionuclide transport. This advantage enables the consideration of phenomenologies not available through TOUGH2.

This work shows how to establish a sequential approach between TOUGH2 and another code. It also presents the conditions of use for such an approach, in terms of performance and the impact of the discretization on the results.

INTRODUCTION

In the course of a performance analysis and safety assessment (PA/SA) of a potential deep geological repository for high-level and intermediate-level long-lived nuclear waste, we must establish ways to simulate hydraulic and gas flow and transport of radionuclides through the repository and the embedding host rock. The PA/SA must consider phenomenologically detailed models, models that describe the flow and transport processes as accurately as possible. This leads to highly nonlinear models, owing to the consideration of such factors as sorption or variable relative permeability. Since the resulting discretized equations have to be solved iteratively, the computational effort is large.

Furthermore, a potential repository is expected to extend over an area of 10 to 20 km^2 and to consist of thousands of emplacement cells, with relevant details at the scale of decimeters. Potential radionuclide release from a repository and transport to the biosphere must be estimated for up to one million years. Consequently, both the spatial and temporal scales represent severe challenges for any numerical modeling approach. Finally, any modern PA/SA includes probabilistic studies to assess uncertainties; for such probabilistic approaches, several hundred or thousand numerical simulations must be performed.

All of the above suggests that fundamental simplifications are required in the course of defining a numerical strategy and solution. One

approach is to simplify the simulations by decoupling the flow and transport computations. The idea is to perform the resource-intensive two-phase flow computation only once, followed by many less demanding single-phase unsaturated transport simulations that reuse the two-phase results. Additionally, the two-phase hydraulic calculation is realized on the coarsest possible discretization in time that would still lead to a reasonable approximation for flow. The discretization for the subsequent transport simulations might be chosen finer, with much less impact on computational time. There are some limitations to this approach, however: The considered nuclides need to be fully soluble in water, and the influence of the nuclides on the flow must be negligible.

The goal of the present work is (1) to implement the aforementioned technique using TOUGH2 for the two-phase flow and the code Traces for the simulation of single-phase unsaturated transport and (2) to study how different discretizations in time for flow and transport simulations impact results. First, we calculate a benchmark two-phase flow and transport and single-phase transport with a very fine discretization. With the discretizations being identical for the two simulations, the decoupling method itself is validated. Subsequently, discretizations are coarsened. The aim of this approach is to meet the benchmark as closely as possible in every calculation using a progressively coarser discretization. This goal is achieved with carefully selected temporal discretizations and interpolation schemes.

The methodology, the construction of a sequential approach, and its application to a simulation case are presented in this paper, followed by a study of the conditions of use for a sequential approach, focused on temporal discretization variation.

METHODOLOGY

The aim of this project is to establish a sequential approach for flow and transport using a hydraulic computation made with TOUGH2-MP with the EOS5 (water and hydrogen) module (hereafter referred to as the T2MP+E5 code). Once this sequential approach is validated by comparison with a reference coupled simulation, the impact of the simplification of the hydraulic data on the transport results is studied.

Decoupling of flow and transport

The first step consists of decoupling the flow component from the transport component of the computation. The computationally intensive two-phase flow field thus needs to be calculated only once and can be used as an input for various transport calculations. For the following decoupled transport calculation, the computational effort is relatively low. This approach can lead to a significant reduction of potentially scarce computational resources when performing the probabilistic studies.

In practice, the decoupled computation is realized in four main steps, as schematized in Figure 1. First, the two-phase hydraulic flow field is calculated. The pore velocity and saturation fields are written as output for every time step by TOUGH2. Then, in order to simulate the transport of the radionuclides, this intermediate output data must be converted into the hydraulic data required by the transport code used in the sequential approach. After this conversion, the unsaturated transport calculation is executed.

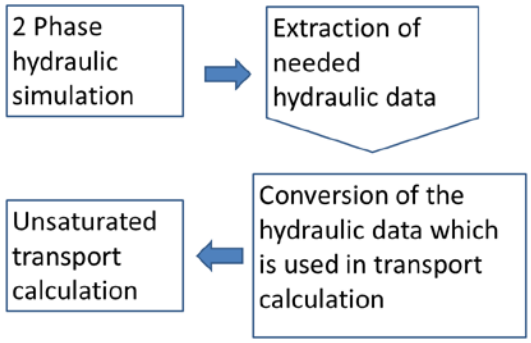

Figure 1. Schematic representation of a decoupled sequential approach for hydraulic and transport simulation.

To validate this method, we perform a coupled two-phase benchmark calculation, and compare the results with those from the sequential approach single-phase transport calculation.

Simplification of the hydraulic data

Once the sequential approach is validated, the hydraulic data required for the transport

computation should be optimized. The work discussed here is a first step towards the separate optimization of the two parts of the sequential approach. This task consists mainly of coarsening the temporal density of the hydraulic data given to the transport computation (Figure 2). Reducing the amount of hydraulic data necessary to run the transport-calculation part is expected to reduce the computation time of the sequence. because processing of flow-field data is minimized.

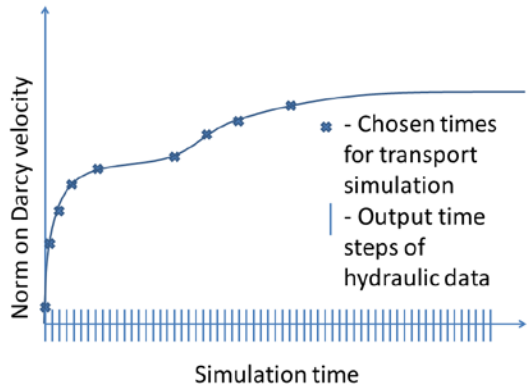

Figure 2. Schematic presentation of the approach to reduce the amount of hydraulic data resulting from the two-phase flow calculation as input for the transport calculation

ESTABLISHMENT OF THE SEQUENTIAL APPROACH

In this section, the setup of a sequential approach is described in detail for simulations modeling the release of radionuclides from an intermediate-level long-lived radioactive (ILW-LL) waste cell, during the resaturation phase occurring after its closure. The gas phase present is hydrogen; hence, T2MP+E5 is used for the flow calculation. For the transport part, we use the one-phase unsaturated transport version of the Traces mixed hybrid finite element (MHFE) code available at Andra.

These results are compared with a coupled reference simulation performed with the TOUGH2-MP EOS75R model, a derivate of EOS7R in which air has been replaced by hydrogen (Kaempfer et al., 2012).

The compatibility between two-phase hydraulics (TOUGH2) and single-phase unsaturated transport (Traces) is monitored carefully, as are the differences between this transport model and the transport model used in EOS7(5)R.

Compatibilities between two-phase hydraulic and unsaturated transport

The mass conservation equation and Darcy's law for the computation of the two-phase flow used in TOUGH2 are described in Pruess et al. (1999). The equation for single-phase unsaturated transport in porous media is formulated according to the Richards model. In the Richards model, the gaseous phase is not modeled, and no exchange between the phases is considered.

Conservation equation for concentration C_i of solute component i per time t – transport equation (Traces):

$$\frac{\partial(R_i\theta_i C_i)}{\partial t} = \nabla\left(\overline{\overline{D_i^*}} \cdot \vec{\nabla} C_i - \boldsymbol{q} C_i\right) + Q_i$$

Here, R_i is the retardation and Q_i the source of component i. To solve the transport problem, the Darcy velocity $\boldsymbol{q}$ and the liquid saturation field are required. The liquid saturation S_l is used to compute the volumetric water content $\theta_i = S_l \cdot \phi$ where ϕ is the porosity. The Darcy velocity is also needed to compute the dispersion present in the diffusion tensor $\overline{\overline{D_i^*}}$. The saturation field is also indirectly used through θ_i to compute the retardation factor R_i, the saturation-dependent dispersion coefficients, and the solubility limits.

The Darcy velocity field in the liquid phase and the liquid saturation field are given by the two-phase hydraulic flow equations. So, physically, there are no inconsistencies between formulating the transport problem either by two-phase flow and transport equations or by a single-phase formulation using hydraulic data from the two-phase simulation—as long as the transport in the gas phase remains negligible. However, inconsistencies may occur because of definition incompatibilities among the variables in the two codes composing the sequential chain.

Creation of two-phase flow data

The results of the two-phase flow calculation are the basic input data for the transport part of the sequential approach, and are therefore generated

for every time step. T2MP+E5 produces the liquid pore velocity (VEL(LIQ)) at the element interfaces and the saturation (SL) of each element in the mesh.

Conversion of hydraulic data

One important step of the sequential approach is to convert the flow data produced by T2MP+E5 into data compatible with transport. In the case of a MHFE code such as Traces, saturation is required at element centers, so the TOUGH2-MP output can be used directly in the transport calculation. The pore velocity, on the other hand, needs to be converted to the Darcy velocity for use by the MHFE transport code. This is done by multiplying the pore velocity by the porosity. The pore velocity is defined at the faces of the element, thus posing the problem of determining the one from among the neighboring elements, the porosity of which is to be used. For two-phase computations, TOUGH2 uses upstream weighting to select the porosity for the computation of the pore velocity from the Darcy velocity. We use the same method.

If mechanical dispersion is considered, Traces also needs the Darcy velocity at the element centers. This is not an issue in this study because we did not consider mechanical dispersion.

Setup of the transport calculation codes

The transport calculation is set up using the generated hydraulic data. Transport-specific parameters must be defined for the Traces code. To be able to compare the results with the EOS75R reference simulation, we must select some equivalent parameters. As a consequence, the differences and incompatibilities between transport in two-phase and single-phase unsaturated (Richards) porous media are studied below.

In terms of processes, TOUGH2-MP EOS75R computes radionuclide transport in the gas phase, which is not possible with the Richards model. However, in the present case, in which we are limited to a radionuclide that remains in solution, transport in the gaseous phase is assumed to be negligible, and this is then not a major incompatibility.

Another limitation of the Richards model described above is the assumption of no temperature dependence of the various properties and parameters. Here we restrict ourselves to an isothermal simulation that serves as a reference. If the influence of temperature on transport is to be accounted for, T2MP+E5 can seamlessly solve the flow problem under non-isothermal conditions. The temperature-dependence of the various transport parameters could be mimicked in Traces by setting up time- and space-dependent parameters that are functions of temperature. EOS75R does not account for precipitation and dissolution of the radionuclides, but this is not an issue in the cases studied here, in which radionuclides with infinite solubility limits are considered.

Other differences stem from the different physical laws employed to model processes and define the parameters:

- Radioactive and decay chains are defined similarly in both models. However, EOS75R is limited to two radionuclides. This limitation is not relevant when tracking the transport of a single radionuclide.
- For retardation, EOS75R considers only the K_d retardation model. The parameters for calculating retardation are defined for every component and material. Other transport codes, such as Traces, also propose other retardation models (Langmuir, Freundlich).
- Diffusion models also have differences. In EOS7(5)R, effective diffusion is defined as $D_{eff} = \phi\tau_0\tau_\beta d_\beta^k$, with d_β^k being molecular diffusion. Three models are proposed (Millington-Quirk, relative permeability, and constant diffusivity) depending on the mode of definition of tortuosity ($\tau_0\tau_\beta$) and d_β^k, whereas in Traces, only constant diffusivity is available. On the other hand, Traces can model dispersion, which is not available in EOS75R. In summary, diffusion models are perfectly compatible between TOUGH2 and Traces as long as the constant diffusivity model is activated in TOUGH2 and there is no dispersion.
- In TOUGH2, porosity is defined by materials in the ROCKS block. Hence it is not possible to define the portion of the porosity

that is accessible by each component, as can be done in Traces. A Traces model equivalent to the TOUGH2 model must be set up accordingly.

- Radionuclide source terms are defined in TOUGH2 EOS7(5)R in kg/s for each element containing a source in the GENER block. Sources can be time dependent. In the particular case of Traces, it is necessary to convert these sources into mol/m^3/s.

Run of the transport simulation

Once all parameters are adequately defined, the Traces model is run, using as input the hydraulic data derived from the T2MP+E5 computation.

APPLICATION OF THE SEQUENTIAL APPROACH

The methodology described above is applied to realize a sequential approach calculation with T2MP+E5 and Traces. Results are compared with a reference coupled calculation performed with TOUGH2-MP EOS75R, which is set up to minimize incompatibilities between the transport parameters, according to the study realized previously.

Benchmark calculation with Couplex-gaz 1b

The benchmark coupled two-phase computation is based on the Couplex-Gaz 1b case (Andra, 2006), which includes simulations of the resaturation period of an emplacement cell of ILW-LL waste. This period starts after backfilling the gallery and lasts till the end of gas production, after 20,000 years. Within the gaseous phase, there are two components, vapor and hydrogen. Hydrogen is transported in the gaseous and the liquid phase. From an extensive geologic analysis it is known that there is an upward-oriented pressure gradient.

The mesh (see Figure 3) uses 2480 elements, among which 80 are boundary elements for the Dirichlet boundary conditions on the bottom and top. The boundaries on the left and right side are no-flow boundaries. The model contains materials with very different hydraulic and capillary properties. For instance, the gap between the concrete and the concrete backfill is modeled as an equivalent porous media material with porosity set to 1.

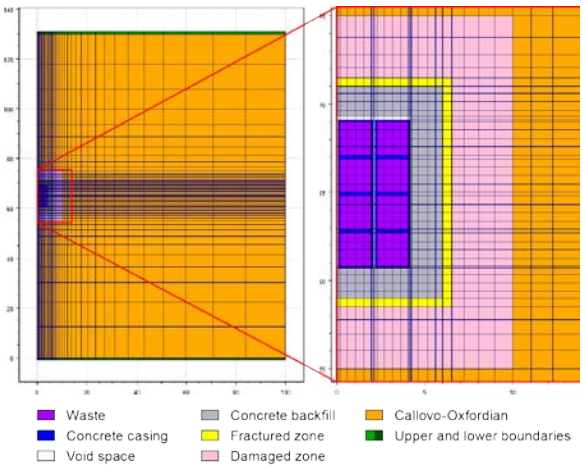

Figure 3. Model domain of Couplex-gaz benchmark case with 2400 elements and 80 boundary elements at top and bottom specified in TOUGH2

A source of I^{129} radionuclide was added in the waste cells with the following production rates:

- $2.5 \cdot 10^{-11}\ kg/s$ from 0 to 500 years.
- $2.0 \cdot 10^{-12} kg/s$ from 500 to 5000 years.

The diffusion model is set to constant diffusivity, in order to be compatible with Traces, and pore diffusion is set to 5×10^{-9} m^2/s.

Performing the sequential approach

The sequential approach is run as described in the previous section. First the two-phase flow transport calculation is run with TOUGH2-MP EOS5. Second, the resulting output data is converted so that finally the transport calculation can be carried out with Traces.

Validation of the sequential approach calculations

The liquid-concentration fields obtained with Traces are compared to the results obtained with the reference TOUGH2-MP EOS75R simulation. TOUGH2 provides these results as a field of mass fraction X_β^k for component k in liquid-phase β, which must first be converted into a concentration field. This is achieved by multiplying the mass fraction by elements volume, density, and porosity, which are also dependent on pressure and temperature by compressibility and expansivity.

Figure 4 shows a comparison of the concentration fields at three different time instants: t= 100 years, t=500 years, i.e., the end of the first phase of I^{129} release, and t=5000 years, i.e., the end of the I^{129} release.

The following observations can be made: First, the concentration fields at all observation times look very similar. There is, however more advancement in the results of the sequential computation, which is particularly visible at t=5000 years. The shape of the concentration plume is very regular, despite the head gradient in the z direction. However, advective transport seems negligible compared to diffusive transport.

To further investigate the differences between the two simulation results, the injected mass and the mobile mass in the model are compared for every output time step. Injected masses in both models are identical, which shows that an adequate conversion of the flow rates was done. However, the mobile mass computed by Traces appears to be slightly high.

Finally, we check that the mobile mass of I^{129} in the gaseous phase within the reference EOS75R calculation is negligible.

We conclude that the quality of the results obtained by the sequential approach is acceptable, taking into account the fact that two very different numerical solutions were used to compute transport.

In terms of CPU time, the reference EOS75R simulation was run in 13,000 seconds on two processors. For the sequential approach, the hydraulic part with T2MP+E5 ran in 2400 seconds on four processors, and Traces in 2450 seconds on one processor. Moreover, the sequential approach required some extra overhead to convert the TOUGH2 hydraulic result into Traces-compatible input files. However, when several transport computations need to be performed with the same hydraulic data, the TOUGH2 simulation and the conversion work necessary for the sequential approach are performed only once. In this case, the Traces transport calculation time is to be compared directly with the CPU times obtained with the coupled TOUGH2-MP EOS75R computation. This illustrates the advantage of the sequential approach in terms of computational speed.

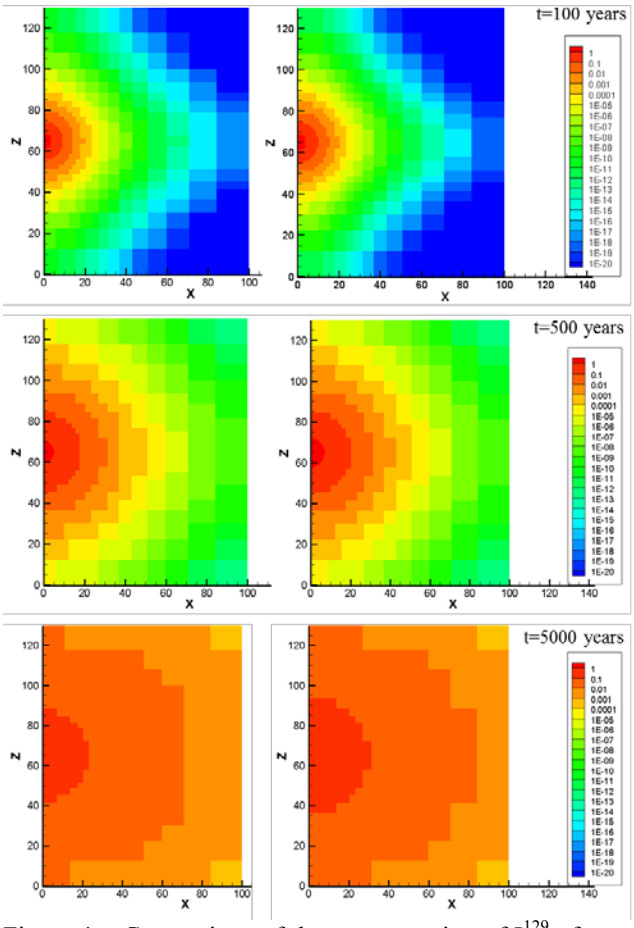

Figure 4. Comparison of the concentration of I^{129} of the reference coupled calculation in TOUGH2 (left) and the sequential approach with Traces (right) for t=100y, t=500y and t=5000y

REDUCTION OF THE HYDRAULIC DATA INPUT FOR SEQUENTIAL APPROACH

In this section, the results of the step involving the simplification of the hydraulic data are presented. As already mentioned, the aim is to reduce the computational effort for one transport calculation by optimizing the amount of necessary hydraulic input data. The process through which appropriate input data are chosen, and the corresponding consequences on the accuracy and the computational performance, are explained in the following paragraphs.

Choice of the time steps from the hydraulic data

The times at which the results of the hydraulic simulation are read into the transport model need to be chosen very carefully. As a criterion for the picking of the relevant time steps, the L_2 norm of the Darcy velocity on all faces of the model domain is calculated for every available time step. This results in a characteristic value for each time step.

The first time step is taken as a reference point. Iteratively, if the relative error, expressed in percentage, of the reference point's norm n_t and the next time step's norm n_{t+1} does not exceed a tolerance threshold tol_{max}, named percentage of tolerance in the following, the latter point n_{t+1} is eliminated. Otherwise, it is selected and becomes the next reference point:

$$\frac{n_{t+1} - n_t}{n_t} < tol_{max} \Rightarrow n_{t+1}\ eliminated$$
$$\frac{n_{t+1} - n_t}{n_t} \geq tol_{max} \Rightarrow n_{t+1}\ selected$$

Only the Darcy velocity and the saturation fields of the selected time instants are used as input for the transport calculations.

Influence of the given input of the hydraulic data on the results of the sequential transport calculations

It must be guaranteed that the accuracy of the results does not suffer from simplifying the time discretization of the hydraulic field data. In order to study the effect of the threshold selection on the percentage of tolerance tol_{max}, the results of the transport of the sequential approach are compared for tol_{max} equal to 1, 2, 4, 8, 16, 32, and 64%. The model is run for these tolerances, and the results are summarized in Table 1 and Figure 5. To compare the results of the simulations, the comparison points are the L-2 norm of the mass fluxes at the top and bottom boundaries of the model domain.

The observation of the results showed that the most significant relative error is found at the top boundary.

Table 1. Time instants, measured computational time and relative error on top boundary of the model for different percentages of tolerance

Number of instants	Percentage of tolerance	Relative error on top boundary	CPU time (s)
2023	0	0.0	2444.8
560	1	3.50E-05	2135.37
364	2	7.74E-05	1971.91
239	4	7.54E-05	1927.43
146	8	1.17E-04	1933.35
91	16	3.20E-04	1550.26
53	32	4.24E-04	1509.49
29	64	1.07E-03	1539.27

The effect of the time discretization on the hydraulic data appears to be very small in this case. This can be explained by the fact that this problem appears to be strongly diffusion-dominated (see Figure 4).

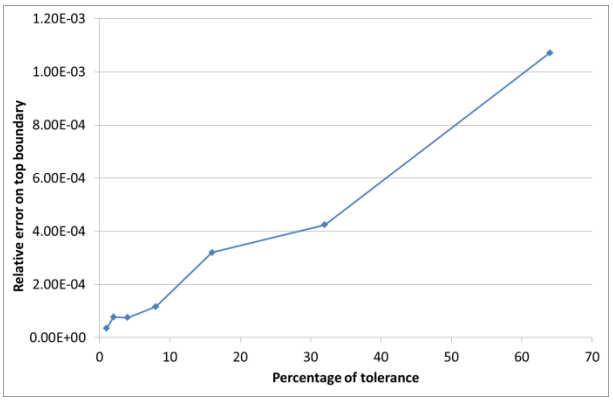

Figure 5. Relative error in fluxes at the top boundary over percentage of tolerance

The computational time is significantly reduced when the hydraulic data provided to the Traces transport code is simplified (see Figure 6). Furthermore, even with a percentage of tolerance on Darcy velocity of 1%, the number of hydraulic times is divided by a factor 4, which is relevant for the production and storage of input and output data.

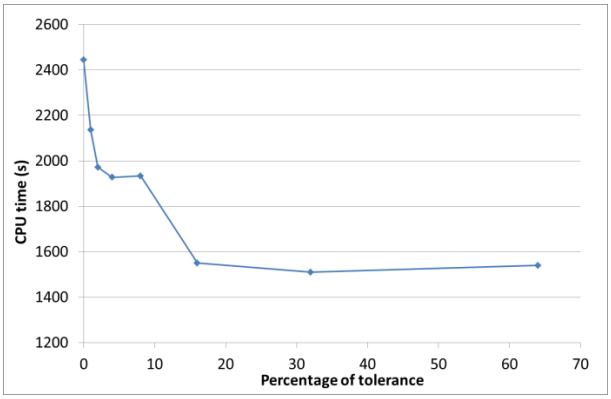

Figure 6. Measured computational time over percentage of tolerance

CONCLUSION

In this work we developed a sequential approach for computing hydraulic and transport in unsaturated porous media and compared it with a coupled two-phase flow coupled hydraulic and transport calculation. In the decoupled calculation, the hydraulic part was computed as a two-phase flow problem solved by the T2MP+E5 code, but for the transport part, the two-phase model was replaced by a single-phase unsaturated transport model (Richards). The study of the two physical models shows that this approach is reasonable under certain conditions, which is confirmed by comparing our results with the coupled and the sequential approach on a Couplex-Gaz 1b based simulation case. The sequential approach has benefits in terms of computation time and also allows the modeler to work around some of the model limitations of the EOS75R model, such as the absence of dispersion or precipitation-dissolution, by using an alternative simulation code for transport.

Gains in terms of CPU time become more significant if the hydraulic data are selected carefully. In practice, the sequential approach will allow modelers to fine-tune the hydraulic and transport simulations separately.

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